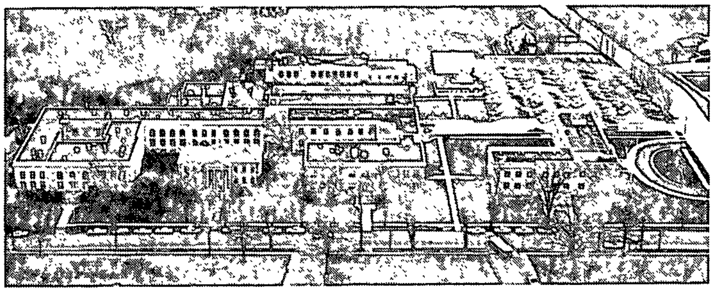

THE INSTITUTE OF PAPER CHEMISTRY, APPLETON, WISCONSIN

IPC TECHNICAL PAPER SERIES

NUMBER 329

NEW DIRECTIONS IN PROCESS SIMULATION

GARY L. JONES

MARCH, 1989

New Directions in Process Simulation

Gary L. Jones

This manuscript is based on results obtained in IPC research and has been submitted for consideration for publication in PIMA

NEW DIRECTIONS IN PROCESS SIMULATION

Gary L. Jones

ABSTRACT

Process simulation must keep up with changes in management philosophy and industry needs. Currently, industries of all kinds are under pressure from foreign competition. The watchword is quality and productivity. Product performance is not only a key factor in maintaining market share, it also affects productivity. If product quality falls below specifications, product must be scrapped or recycled resulting in delays, lost production, and increased energy consumption.

Steady state process simulation has been a useful tool in the past to provide detailed mass and energy balances for process design and to make incremental improvements. Dynamic simulation is useful for training and process control. Combined with optimization techniques, simulation can also be used to optimize process conditions, develop improved designs, and reconcile on-line data measurements.

However, until recently, process simulation has not provided information on product quality or so-called end-use performance. To ignore product quality would be like calling the paper roll at the end of the machine nothing but tons of fiber, fillers, and moisture. These factors must also be factored into the design. It is common practice to design a new machine or mill based primarily on throughput and energy criteria without determining the grades to be produced. The result is a long period of product shakedown and rearrangement of product lines across numerous machines after the new mill or machine is brought on stream.

Process simulation, which could predict product quality, would be useful as part of the process design sequence to minimize these types of problems. It could also be very helpful in troubleshooting certain types of product quality problems, or to assess the impacts on quality of various changes in the mill. It could also be used to develop optimal conditions not only from the standpoint of throughput and energy, but also product quality. Ultimately this system could be used as part of a process control system on-line to close the loop between sophisticated sensors and the variables to be manipulated.

A prototype system to simulate a wide range of quality factors for paper has been implemented in MAPPS. The paper will describe how process conditions from the wood yard to the calender affect the fibers and the network and ultimately affect product quality. Applications of the system are used to illustrate how it would be useful in design, troubleshooting, and optimization.

BACKGROUND

Simulation in its various forms is now a widely applied technique throughout the U.S. economy. However, the variety of its uses almost defies a good definition. Viewed in a broad context, simulation could be referred to as any result of a computation of an activity or process. There are many dimensions in the simulation world. One of great importance is time. Dynamic simulation is the most widely used and has the highest economic value. It's used for training, and control places it in the most critical location at the man-machine interface.

Another dimension which distinguishes various simulation activities is the granularity or the degree of parameter lumping as shown in Figure 1. At the very highest level of lumping, we would put an economic model of the U.S. economy. Lower levels of lumping or breadth are required for process models. Highly granular simulations such as detailed flow or structural mechanics calculations using finite difference or finite element programs (FLUENT or FIDAP) are very limited in breadth. Chemists now perform molecular simulation which represents the ultimate in granularity currently available.

GRANULARITY

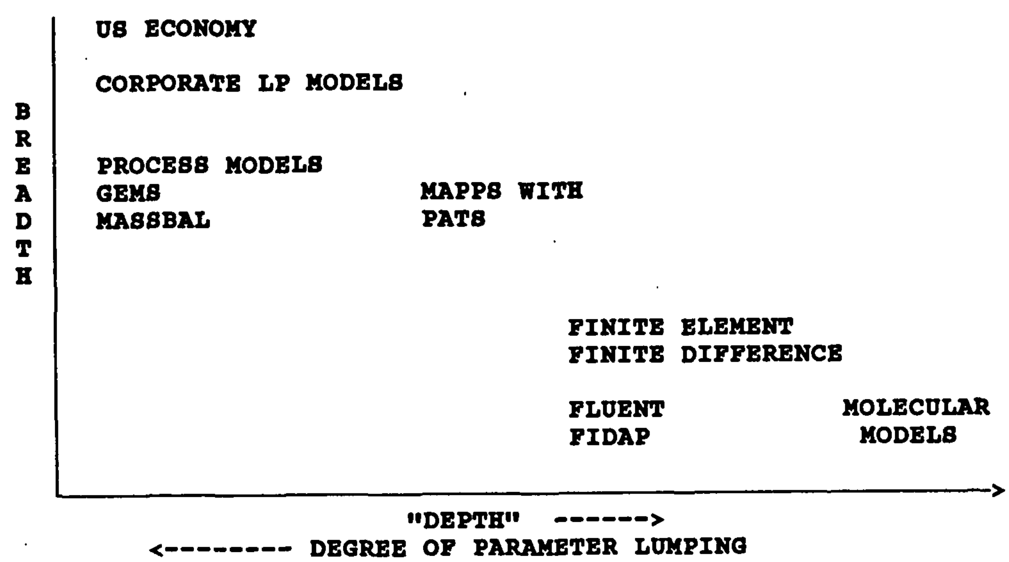

Figure 1

One problem with the "deeper" programs is that information from them is far too detailed and specific, and must first be lumped into useful bites and displayed in a simpler format. Once this is done, the "deeper" programs can provide information available in no other way except through experimentation.

Although there appears to be a tradeoff between breadth and depth, it is possible to achieve more depth without a large sacrifice in breadth. The most widely-used process simulation programs in the pulp and paper industry, GEMS, MASSBAL II, and MAPPS, are designed for a broad range of process calculations, but usually provide very little detail about any one process. Note, however, that MAPPS lies at the same level of breadth but to the right in an area of greater depth. The difference is a new dimension in simulation called performance attributes or PATs.

Performance attribute modeling is a novel extension of the MAPPS mass and energy balance program with the potential to revolutionize decision-making in pulp and paper manufacturing. PAT modeling links the processing stages applied to well-characterized raw materials to predict the resulting attributes of paper required for use in a variety of products.

Benefits of Attribute Modeling

The ability to balance raw materials and processing steps to produce paper with a given end-use capability offers a host of opportunities for optimization of the paper manufacturing process, including significant opportunities for reduced energy consumption in an energy-intensive industry. Some of the potential benefits with energy implications include reduced energy consumption through increased use of recycled and high yield furnishes, reduced fiber loss in manufacturing, reduction of off-specification product, and subsequent recycle and optimized processing steps for a given product specification. It also includes improved decision-making in process and capital equipment selection.

How Depth is Achieved Through Attribute Modeling

PAT's add depth to the traditional mass and energy balances by representing through models fundamental properties of fibers and the networks which form paper. These models make it possible to simulate the pulping and papermaking processes with greater depth. New, more predictive and easier-to-use models of the paper machine, wet presses, calenders, screening, cleaning, and refining systems are then developed using the fiber and network models. Finally, the fiber and network models are combined to predict various sheet properties which are measures of end-use performance. With PATs, depth is achieved and the information is provided in a useful form for decision-making.

Property Development During Papermaking

Paper manufacture begins with chips from one or more species, and ends with a dozen of grades with hundreds of end-use performance characteristics or specifications. In between, the fibers are separated, processed to enhance their bonding potential, formed into sheets, pressed to consolidate and remove water, and dried and passed through a variety of converting operations to achieve the final slate of properties.

Conventional process simulation techniques treat this process as a flow of mass and energy. Fibers are viewed simply as lumped components of cellulose and lignin or as generic fibers. Neither the structure of the fibers nor the network is represented. Important interactions between fiber or network properties and mass and energy balances, particularly in sheet forming and dewatering, were also impossible to represent with the conventional approach.

Basis for the PAT Models

A considerable body of knowledge has been developed relating characteristics of fibers and the developing network with the final sheet properties. Until recently, this information was underutilized and almost totally lacking in process simulation and modeling.

Early work by a committee of TAPPI showed that sheet properties could be related to a handful of fiber variables[1]. Similar conclusions have been drawn by many others[5,9,10] as well as by studies at IPC[2,28]. Many have contributed to establishing a theoretical framework of the structure of paper and models of many sheet properties[3-12,14-23]. Relevant areas of fiber and sheet structure, optical properties, and process effects have been extensively reviewed[8,9]. Others have contributed knowledge on the wide variety of factors which influence fiber and network properties such as species, sheet forming, web consolidation, stretch, orientation, and pulping[13,24,25]. Others have helped define key performance attributes[26,27].

OVERVIEW of the PAT SYSTEM

Figure 2 illustrates the interactions between mass and energy balance models, PAT models, and property models. The models are input-output in nature so the mass and energy flows and attributes leaving a processing step are changed depending on the characteristics of the processing step. Attributes of the entering and leaving streams along with material flow information are used to determine properties of the streams entering and leaving each operation block.

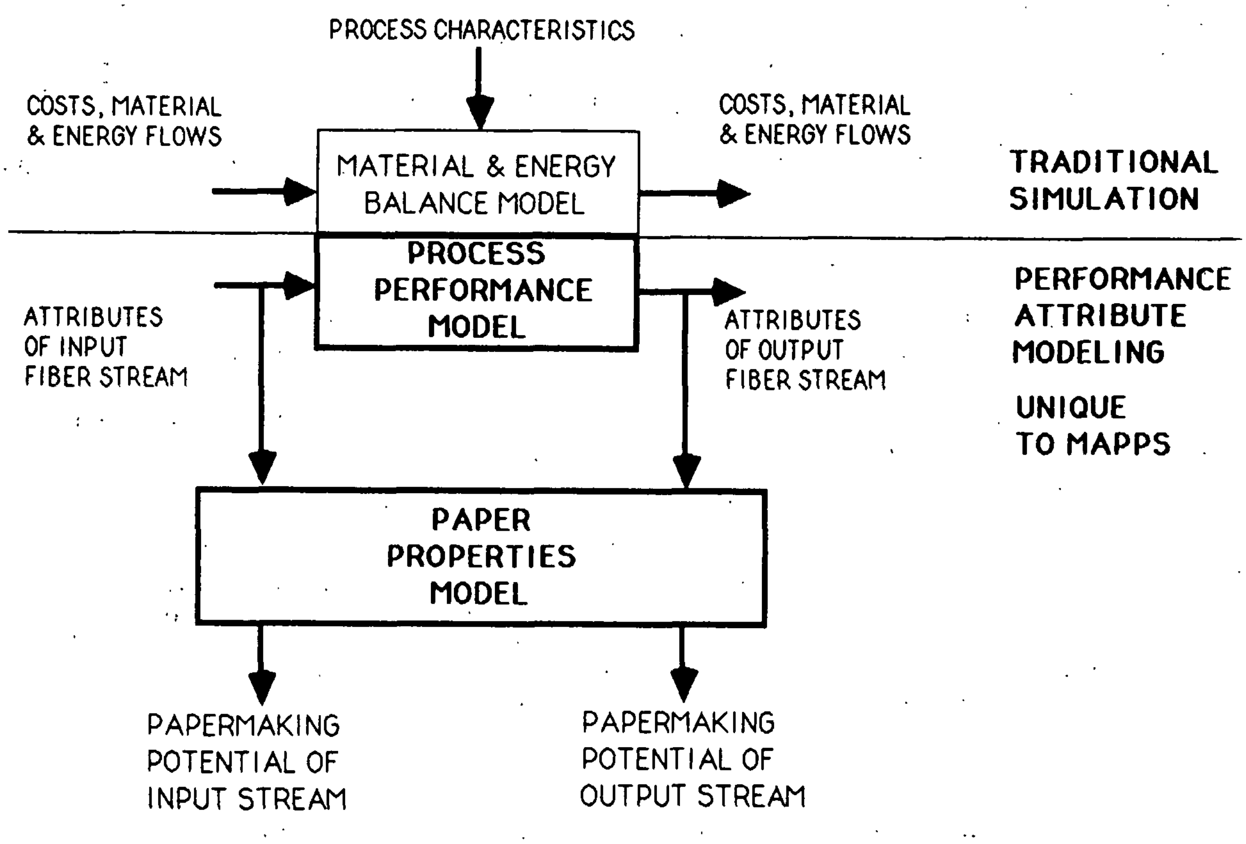

Figure 2

A process flowsheet model made up of many individual process blocks is constructed to simulate the process. Simulation with the process model then provides information on the development of properties and attributes throughout the process as illustrated in Figure 3.

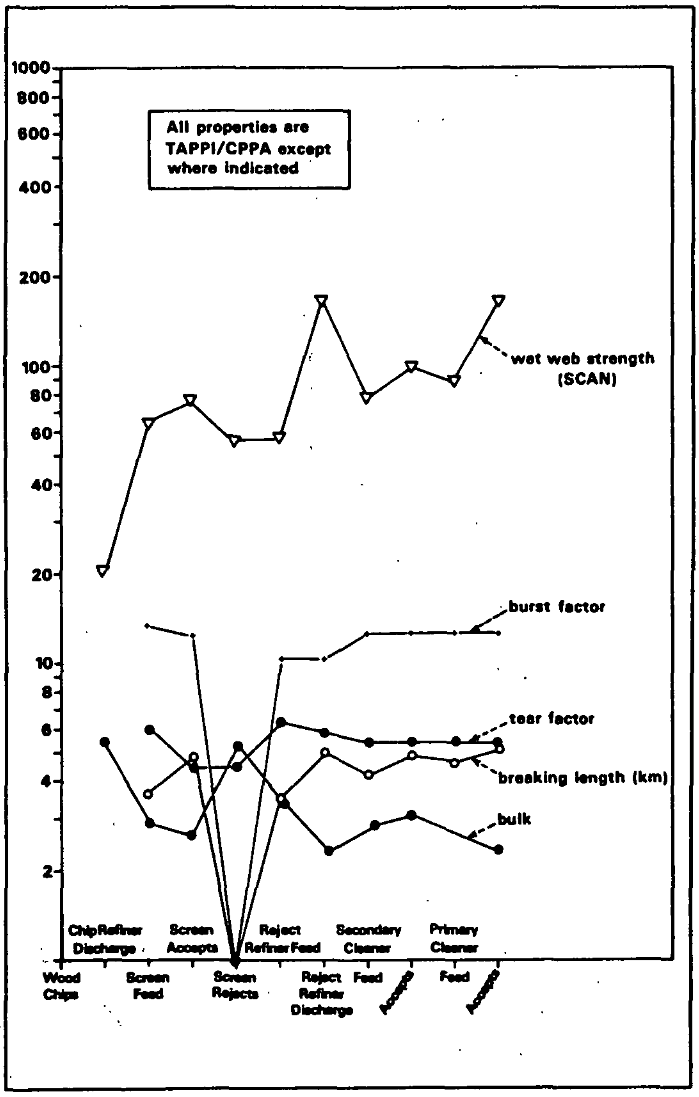

Figure 3

The PAT system accounts for a wide range of operations which influence end-use properties such as species, pulping, screening, cleaning, bleaching, additives, sheet forming, wet stretching, wet pressing, drying, calendering, and repulping. Species is accounted for through a species data base. The remaining operations are accounted for through models of the effect of each process on specific performance attributes. Although not discussed here, the PAT system has brought about an expansion in the power of the processing models. For example, new models of the forming section (Fourdrinier), wet presses, calenders, refiner, stock prep, and bleaching areas, have been developed using PATs.

Figure 4 shows how PAT's represent various aspects of fibers and network which form paper.

OVERVIEW OF PAT SYSTEM IN MAPPS

PAT'S			
Yield Kappa Xhemi C_k	Composition	FIBERS	PAPER
L, σ_l W, σ_w JDIST CWT	Morphology	FIBERS	PAPER
Density Tensile Modulus Flexibility factor	Physical	FIBERS	PAPER
K-factor CSF	Surface area	FIBERS	PAPER
S_{p1}, S_{p2} (sidedness) S_a	Bonds	NETWORK	PAPER
Formation factor Wet Strain Orientation	Anisotropy	NETWORK	PAPER

Figure 4

Composition Attributes

Fibers consist of alpha-cellulose, amorphous or hemicelluloses, lignin, extractives, and ash. However, for convenience the attributes used to represent fiber composition are yield, kappa number, and the ratio of hemicellulose to total cellulose. With these variables it is possible to determine the actual fiber composition no matter what form the components may have throughout the process.

Shape Attributes

Fiber shape is represented by fiber length and width distributions and cell wall thickness. Each distribution is represented by the average and the standard deviation. A third parameter defines the type of distribution, i.e., log-normal, normal, or Weibull. By combining the distribution functions to form a matrix, it is possible to represent all combinations of length and width. The matrix is used to compute the fibers, fines, and shives measured with screens or fiber analyzers.

Fiber Physical Property Attributes

Physical properties such as fiber density, tensile strength, and tensile modulus are extremely influential in determining final sheet properties. These attributes are initialized by the data base and changed in pulping, bleaching, and refining operations.

Fiber Surface Area Attributes

External surface area is developed extensively by refining, and is a critical step in papermaking. The first attribute in this category is Canadian Standard Freeness, CSF, which is a direct measure of external surface area.

The second attribute is the K-factor which represents the fibrillation generated by refining. For a given fiber length distribution and K-factor, it is possible to compute the hydrodynamic specific surface area. A second relationship relates CSF to hydrodynamic specific surface.

The two important effects of refining, fiber separation, and surface area development, are accounted for through the use of fiber distribution parameters, K-factor, and CSF. Other effects such as swelling, fiber flexibility, and bonding potential are accounted for by other factors discussed later.

Optical Attributes

The light absorption coefficient is an inherent characteristic of the lignin color bodies in the fiber. This attribute is influenced by lignin removal steps such as pulping and bleaching. A second factor, light scattering, can be predicted from other sheet characteristics. Sheet brightness, an important end-use performance characteristic of many grades, can then be predicted from absorption and scattering.

Brightness development is accomplished through various types of bleaching operations. Bleaching can also have other beneficial effects on other properties through the removal of lignin. The three attributes, yield, kappa, and absorption coefficient, can be used to account for the main effects of bleaching.

Fiber Stiffness Factor

Bonding potential is strongly related to fiber bending stiffness. Most factors affecting fiber stiffness such as cell wall thickness, yield (more lignin present), and degree of refining (less swelling or removal of the outermost layer of the fiber) are already accounted for through three attributes previously mentioned. The remaining influences are lumped into the fiber stiffness factor which is used to account for stiffening during drying and the effects of reslurrying and secondary fiber reuse.

Network Formation

Once the fibers have been separated and their surface area and flexibility developed through refining, the stage is set for network formation. The sheet forming process, such as the Fourdrinier, handsheet former, or twin wire former, forms a mat of fibers and separates water from the mat. Inevitably, much of the fine fibers and suspended material pass with the water. The PAT system determines the attributes of the mat and of the white water draining from the mat throughout the forming process.

The network forms as fibers make contact during drainage. Contact area is related to the specific surface available and the fiber flexibility as shown at the top of Figure 5. As fiber retention changes during drainage, fiber contact area varies throughout the thickness of the mat. Contact area attributes S_{p1} and S_{p2}, for the top and bottom of the sheet, represent the developing network.

As the web is densified during wet pressing, these contact areas increase as shown at the bottom of Figure 5. The increase depends on the web compressibility which in turn depends on other attributes such as cell wall thickness, composition (yield), and freeness. During drying, hydrogen bonds form at the contact areas and the contact areas are converted to fiber bonded area.

BOND DEVELOPMENT MODEL

- Fiber Property and Early Network Development

Hydrodynamic Specific Surface + Fiber Flexibility --------> (Forming) Fiber Contact Area (S_{p1}, S_{p2})

Refining, Species → Hydrodynamic Specific Surface

Refining, Pulping, Species → Fiber Flexibility

- Sheet Consolidation and Bond Formation

Fiber Contact Area ---------> (Pressing) Fiber Contact Area -------> (Drying) Fiber Bonded Area

Fiber Flexibility → Pressing

Figure 5

As illustrated in Figure 6, contact area and the fiber geometry determine sheet density. Bonded area, fiber geometry, and formation determine bond density. For a dry, well-formed sheet, bond density is equal to sheet density and the well-known correspondence between tensile and elastic properties and sheet density follow. However, when the sheet is not well-formed, or when operations such as calendering break bonds, the relationships change.

DENSIFICATION AND STRENGTH DEVELOPMENT

contact area	**+ fiber geometry**		**----->**	**sheet density**
bond area	**+ fiber geometry**	**+ formation**	**----->**	**bond density**
bond density	**+ fiber strength**		**----->**	**tensile properties**

Figure 6

Sheet Structural and Tensile Anisotropy

A sheet of paper is not perfectly uniform. Paper varies structurally from point to point. Paper properties also vary due to nonuniform stress distribution in the sheet. The three types of anisotropy accounted for in the PAT system are formation, tensile anisotropy due to fiber orientation and sheet stretch during drying, and sidedness due to nonideal retention and fiber laydown during forming and consolidation.

Tensile Anisotropy

Fibers tend to be oriented preferentially in the machine direction during forming, and as the sheet is preferentially strained in the machine direction. Both of these processes lead to directionally dependent properties in all three directions, MD, CD, and ZD. Tensile anisotropy is accounted for through the fiber orientation and wet stretch attributes.

Z-D Variability - Sidedness

The variability throughout the thickness of the sheet (Z-D), is accounted for by the use of the fiber shape and surface area attributes. As each layer of the sheet is formed, this information is stored in the Z-D variability array. The array can then be used to determine the degree of fiber contact and the bonded area on each side of the sheet. Sidedness and Z-D variability affect sheet properties. For example, for many forming methods, the topside will be denser, smoother, stronger, more bonded, and have lower scattering than the wire side.

Formation

Formation relates to the spatial variation (mainly M-D and C-D) in the distribution of fibers. This may be quantified as a variation in sheet basis weight and caliper, or more simply as a variation in sheet density. Formation is determined by the forming conditions and the characteristics of the stock (particularly fiber length and freeness). Poor formation leads to poor tensile properties and a poor visual appearance. Differences in formation between handsheets and machine paper make the prediction of machine paper from handsheet data a difficult task. Direct prediction of machine paper quality would, therefore, be very beneficial.

The formation efficiency factor, (see Figure 4), represents the coefficient of variation or efficiency of bond formation. It is not to be confused with formation as measured optically. Low density areas represent areas of low bond density. The converse is true of high density areas. Because the ultimate strength of the network is governed by the weakest members, the effective bond density is reduced as the formation factor drops below its ideal value of 1. This results in a weaker sheet. Other things being equal, longer fibers will exhibit lower formation efficiency than shorter fibers. The effective bond density and sheet tensile will be lower when formed on a paper machine than they would be if formed on a handsheet mold. Formation efficiency also decreases with increasing forming consistency and jet-wire speed ratio.

Other Factors

The sheet structure can be altered in a variety of ways during papermaking. Strength or retention aids can be added before the sheet is formed to alter fiber bonding or fines content. Fillers are added to increase opacity by occupying space between fibers. Coatings are applied to alter sheet surface properties. Multiple sheets are formed to produce a composite structure with unique properties. At the present time, these effects are not accounted for by the PAT system. However, there is no reason they could not be added at a later date.

Many other operations are handled by the PAT system. For example, reslurrying of the paper is the reverse of drying. Adding water to the sheet reduces bond area and bond density with a reduction in strength. Low levels of moisture can reduce strength without reducing bulk density. Sheet properties can be altered through converting operations. Calendering represents the most common and important converting process. Different calendering methods are used depending on the grade and forming method.

Sheet Properties

There are hundreds of important sheet properties depending on the grade and end-use. Properties computed by the PAT system are broken down into general categories as shown in Table 1.

TABLE 1
SHEET PROPERTIES

Density Porosity	Structural
Young's Modulus Directional Moduli	Nondestructive
Breaking length Stretch Burst, Tear, TEA Directional Tensile Compressive Strength	Destructive
Scattering, Gloss, Roughness Brightness Opacity Smoothness/Roughness Scott Bond	Surface Optical Printing

APPLICATIONS

To illustrate use of the PAT system, a bleached kraft mill pulping longleaf pine was simulated. The pulp was refined to varying freenesses from 325 to 550. Handsheets were made at different wet pressing pressures from 0 to 60 psi. The handsheets were then reslurried and lightly refined and reformed into handsheets to determine the effect of densification conditions on the repulped fibers. Results for three representative properties, density, burst, and tear are shown for the virgin pulp and the effects of six repulpings in Figures 7-9. The effects as one might expect are complex. The relationship between strength and density depend on the densification conditions used.

The effects of repulping are similar to those seen between fibers of different wall thickness. Thus the differences shown between virgin fiber and six repulpings mimic the differences between or within species of different fiber wall thickness. For a variety of species, the effects of six drying cycles are equivalent to a 50% increase in cell-wall thickness. Although not shown in the figures, increasing yield from 47 to 100% shifts the lines downward and increases the response to pressure and freeness.

Figure 7 shows that sheet density increases with wet pressing pressure and refining (decreasing CSF). The response to refining or pressing is different at various levels of the other due to mat compressibility and fiber flexibility interactions. The effects of multiple repulping are shown by comparing lines marked virgin fibers (zero repulping) with lines marked six repulpings. Repulping tends to stiffen fibers, which reduces sheet density at normal pressures of 60 psi, but leads to a small increase at zero pressure and low refining levels (500-600 CSF).

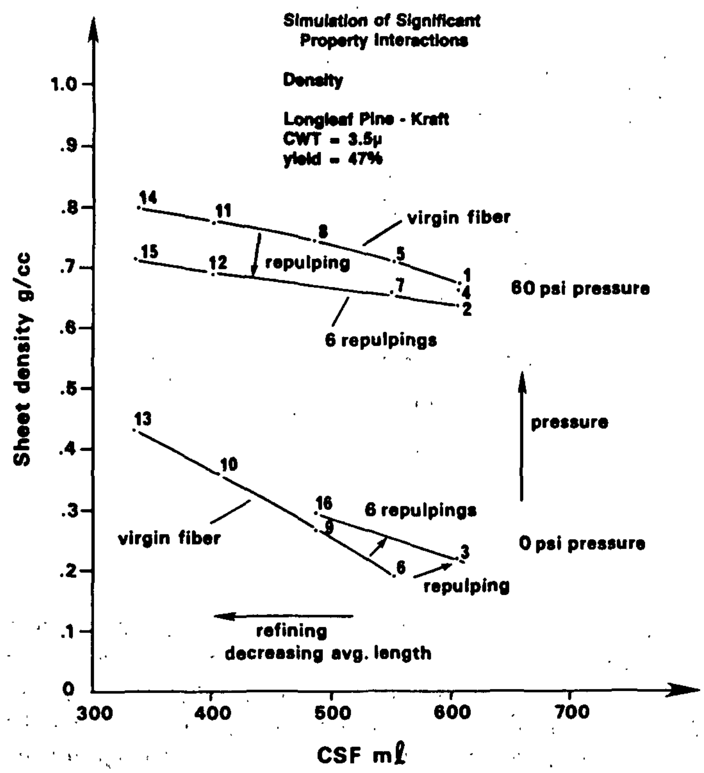

Figure 7

Figure 8 shows the response of burst factor to density for various levels of pressure and repulping. Increased refining and pressure leads to an increase in burst and the response to each varies with the other. Repulping tends to reduce burst, as it does with most tensile properties. However, the effects of repulping on burst can be partially overcome by refining and pressing.

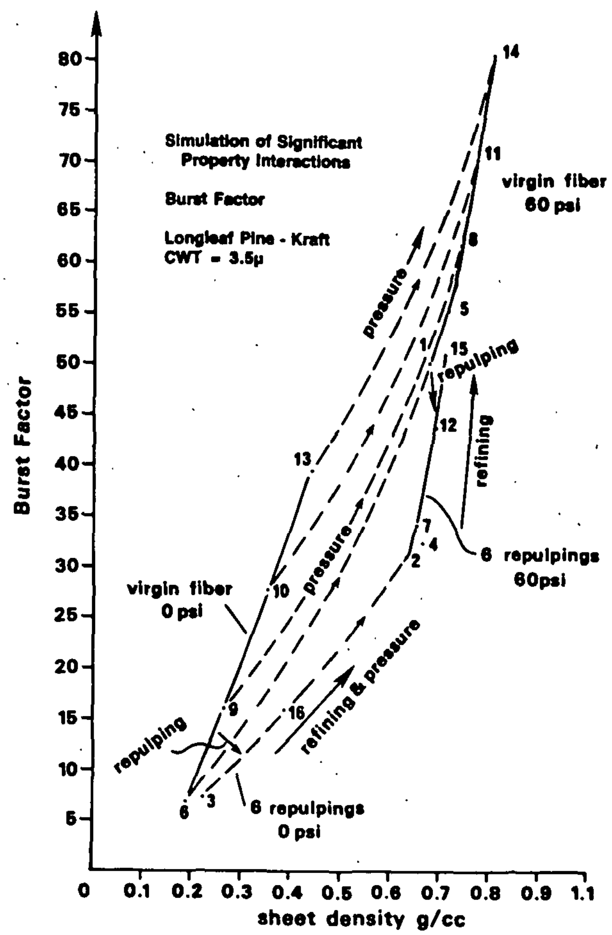

Figure 8

Figure 9 shows tear factor which tends to respond in the opposite direction to burst factor. However, tear is also more dependent on fiber length than either density or burst. For repeated refining cycles, fiber length tends to decrease, which decreases tear factor. Tear is not very sensitive to pressure, but is highly sensitive to refining. The effect of repulping varies significantly with pressure, however. At low pressure, repulping tends to decrease tear, while at higher pressure, repulping tends to increase tear.

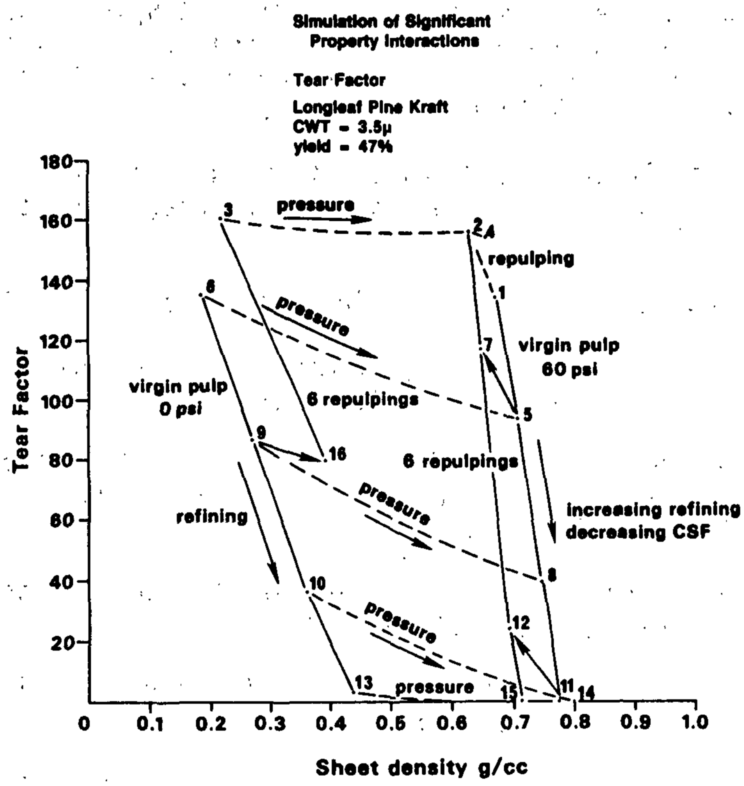

Figure 9

Other applications include property development in a TMP mill using the MAPPS PAT system to be published in an upcoming issue of Pulp and Paper Canada and simulation of a newsprint mill with bleached kraft, semibleached stone groundwood, and paper machine to be presented at the TAPPI Engineering Conference in Fall 1989. The potential applications are essentially limitless.

CONCLUSIONS

The PAT system promises to enhance the benefits of simulation by making it possible to couple product property development to the mass and energy consumption. This new capability should also make it easier for engineers to perform calculations from realistic data, rather than arbitrary splitting and mixing as in the past. Ease of use is a key factor and must play an important role in the form the system takes. The potential is great for expanding the depth as well as the breadth of simulation output to provide a wider range of information to make the job of the engineer and manager easier.

REFERENCES

1. "Quality Control in the Forest and in the Mill, A Systems Approach to the Impact of Tree Breeding, Forestry Practices and Mill Technology on the Quality of Linerboard and Multiwall Sack Paper Made of Southern Pine Kraft Pulp, CA Report No. 54, TAPPI Press, (1974).

2. Jones, G. L., "Simulating the Development of Pulp and Paper Properties in Mechanical Pulping Systems," Pulp and Paper Canada, 89(6):128-30, 132-4, 136-8 (June, 1988).

3. Habeger, C. C. and Whitsitt, W. J., Fibre Sci. Technol. 19:215-239 (1983).

4. Sprague, C. H. and Whitsitt, W. J., "Compressive Strength Relationships and Their Evaluation," Tappi 65(12):104-105 (1982).

5. Alexander, S. D., Marton, R., and McGovern, S. D., "Effect of Beating and Wet Pressing on Fiber and Sheet Properties I., Individual Fiber Properties." Tappi 51(6):277(1968).

6. Baum, G. A. and Bornhoeft, L. R., "Estimating Poisson Ratios in Paper Using Ultrasonic Techniques." Tappi 62(5):87(1979).

7. Baum G. A., Brennan, D. G., and Habeger, C. C., "Orthotropic Elastic Constants of Paper." Tappi 62(8):97(1981).

8. Bristow, J. A. and Kolseth, P., Paper Structure and Properties, International Fiber Science and Technology Series/8, Marcel Dekker, Inc., NY (1986).

9. Clark, J. d'A, "Pulp Technology and Treatment of Paper," Miller Freeman, San Francisco, (1978).

10. Dinwoodie, J. M., "The Relationship Between Fiber Morphology and Paper Properties: A Review of Literature." Tappi 48(8):440(1965).

11. Fleischman, E. H., Baum, G. A., and Habeger, C. C., "A Study of the Elastic and Dielectic Anisotropy of Paper." Tappi 65(11):115-18(1982).

12. Habeger, C. C. and Whitsitt, W. J., "A Mathematical Model of Compressive Strength of Paperboard." Fiber Sci. Technol. 19:215-329 (1983).

13. Han, S. T., "Compressibility and Permeability of Fibre Mats," Pulp Paper Mag. Can. 70:T134(1968).

14. Higgins H. G. and de Yong, J., "The Formation and Structure of Paper," Transactions of Oxford Symposium 2:651(1962).

15. Kellogg, R. M., Thykeson, E., and Warren, W. G., "The Influence of Wood and Fiber Properties on Kraft Converting-Paper Quality." Tappi 58(12):113 (1975).

16. Malmberg, B., "Relationships Between Properties in Laboratory Hand Sheets. Part 1. Softwood Pulps." Svensk Papperstid. 3(15):69(1964).

17. Malmberg, B., "Relationships Between Properties in Laboratory Hand Sheets. Part 2. Hardwood Pulps." *Svensk Papperstid. 3(16):617(1964).*

18. Nissan, A. H. and Battan, G. L., Jr., "Unification of Phenomenological, Structural and Hydrogen-Bond Theories of Paper, Using Percolation Concepts." Nordic Pulp and Paper Research Journal 1987:8-14.

19. Page, D. H. and Tydeman, P. A., "A New Theory of the Shrinkage, Structure, and Properties of Paper." Transactions of the Symposium of the Technical Section of the British Paper and Board Makers Assoc., Oxford, 1:397(1961).

20. Page, D. H., "A Theory for the Tensile Strength of Paper." Tappi 52(4):674(1969).

21. Page, D. H., Seth, R. S., and De Grace, J. H., "The Elastic Modulus of Paper. I. The Controlling Mechanisms." Tappi 62(9):99(1979).

22. Van den Akker, J. A., Lathrop, A. L., Voelker, M. H., and Dearth, L. R., "The Importance of Fiber Strength to Sheet Strength." Tappi *41(8):416-25(1958).*

23. Van den Akker, J. A., Structure and Tensile Characteristics of Paper." Tappi 53(3):338(1970).

24. Setterholm, V. C. and Chilson, W. A., "Drying Restraint - Its Effect on the Tensile Properties of 15 Different Pulps." Tappi 48(11):634(1965).

25. Setterholm, V. C. and Kuenzi, E. W., "Fiber Orientation and Degree of Restraint During Drying - Effect on Tensile Anisotropy of Paper Properties." Tappi 53(10):1915(1970).

26. Strand, B. D. and Edwards, L. L., "Optimum Design, Operation and Control of Mechanical Pulping Systems." Tappi J. *67(12):72-5(1984).*

27. Yan, J. F., "Kinetic Theory of Mechanical Pulping." Tappi 58(7):156-8(1975).

28. Jones, G. L., "Simulation of the Performance Characteristics of a TMP Mill," to be published in Pulp and Paper Canada, 1989.